In the claims:

Please amend claims 8 and 13-14 as shown in the attached clean and marked forms of the pages showing the claims as now pending, pursuant to 37 C.F.R. 1.121(b).

REMARKS

The applicant responds to the final Office Action dated December 4, 2001, and overcomes each of the office action's grounds for rejection of the claims.

Claims 8 and 13-14 have been amended. According to an aspect of the invention, fixed bond information is derived. A delocalized representation of a chemical structure is analyzed. Based on valence information, a plurality of fixed bond representation candidates are identified for at least a portion of the chemical structure. At least a subset of the fixed bond representation candidates are evaluated. A selection is made from among the plurality of fixed bond representation candidates based on the evaluation.

Rejections Under 35 U.S.C. 112

Claims 1-18 have been rejected under 35 U.S.C. 112, first paragraph, as containing new matter. The action refers to the claim language "selecting from among the plurality of fixed bond representation candidates based on the evaluation" and states that "the applicant does not clarify what this evaluation will consist of". Applicant respectfully disagrees with the rejection. Applicant asserts that the originally filed disclosure supports the "based on evaluation" claim language and that there is no new matter, even if the specific word "evaluation" has not been found in the specification. As stated in MPEP 2163.02, "[t]he subject matter of the claim need not be described literally (i.e., using the same terms or in haec verba) in order for the disclosure to satisfy the description requirement." In fact, the specification is replete with examples of evaluative actions, including examples indicated by the terms underlined in the following excerpts of the specification at pp. 5-10:

Conceptually, in a specific embodiment of the procedure, a path is traced through the structure and, for each atom, each possible electronic and bonding state is examined that is consistent with previous results along the path. By extensively or exhaustively examining possible states and orders, the procedure is able to arrive at a fixed bond solution, if one exists.

...

All possible ESVDs may be attempted for all atoms, and all bond orders (including single and double) may be attempted for all bonds. A solution is determined to have been found when a combination of codes and orders is self-consistent, such that, for every atom, the orders of bonds to the atom match the requirements of the atom's ESVD, and the net charge and number of paired electrons of the system are also as required by the structure. Possible further requirements include a satisfactory 4n+2 electron count or an absence of radicals or zwitterions.

In a specific implementation, the procedure includes several practical features that help to produce timely results in practice. A first of the practical features reflects a recognition that it is not always necessary to try all ESVDs and bond orders: with respect to choosing an order for a bond to an atom having an assigned ESVD, the only orders considered are orders that are consistent with the ESVD, taking account of bonds already assigned. For example, if a carbon ([121/1]) has been assigned a double bond, the carbon's next bond may not be double, and is only considered to be single. Further, the only ESVDs that are chosen are ESVDs that are consistent with adjacent fixed bonds.

A second of the practical features is consistent with a recognition that in practice many or most solutions do not involve unpaired electrons or charge: ESVDs featuring unpaired electrons or charge are not considered initially. If a solution is found without referring to such ESVDs, the procedure is finished, and time has been saved.

According to a third of the practical features, the procedure is only partially recursive. With respect to bond orders, when alternative bond orders are attempted, recursion is sensible: if a single bond appears to be the most advantageous next step, and its recursive development returns in failure, the double bond remains the most advantageous next option. In other words, pursuit of a bond order is exhaustive. By contrast, with respect to ESVDs, some ESVDs tend to be more promising (i.e., better) than others, in at least some cases. Accordingly, after the possible ESVDs for an atom are tabulated, the best of the possible ESVDs is actually

pursued, recursively, and the rest of the possible ESVDs are placed in a priority queue, keyed to a rating of the inchoate structure's likelihood of success. In this way, less promising ESVDs are not examined until more promising combinations are exhaustively considered.

Another of the practical features in a computer-based implementation is an implementational measure that speeds the assessment of compatibility between bonds and ESVDs: a screening bitmask. (A bitset is a piece of data, e.g., an integer, in which each bit represents a Boolean value. As used herein, a bitmask is synonymous with a bitset.) For a given ESVD, a screening bitmask encodes the ESVD's bonding and electron requirements. Similarly, for an atom, another screening bitmask specifies which types of bond have already been fixed. When the latter screening bitmask is logically (i.e., bitwise) subtracted from the former screening bitmask, a list of bond types still required at the atom is obtained. By logically subtracting the former screening bitmask from the latter screening bitmask, it can be determined whether it is possible to apply the ESVD to the atom. Such operations tend to save time, since multiple logical comparisons are compressed into one comparison of bitmasks.

In a specific implementation, the screening bitmask for the ESVD [121], for example, can be figured from Table 3 (Fig. 11). Only the bonding portion of the bitmask is considered when choosing the bond orders compatible with an ESVD. The internal single bond, the internal double bond, and the external single bond of the ESVD [121] correspond to bits #0, #2, and #4, respectively. Therefore, the bitmask has the value {0,2,4}. For an atom that has had one single bond fixed, the bitmask consists of bit #0, with the value {0}. The difference between the former and latter bitmasks, {0,2,4} - {0} = {2,4}, reveals the fixed bond types that must eventually be assigned to the atom, namely, an internal double bond (bit #2 and an external single bond (bit #4).

An example of the opposite process is determining whether an ESVD, such as [111/2-], is compatible with an atom that, for example, has two fixed single bonds and which, due to a global restraint, may not be charged. The ESVD's bitmask is {0,1,4,10,12,14}, indicating that the ESVD has an internal single bond, has two internal single bonds, has an external bond, is negative, is not positive, and does not have an unpaired electron, respectively. The atom's bitmask is {0,1,8,11,12}, indicating the atom has an internal single bond, has two internal single bonds, is neutral, is not an anion, and is not a cation, respectively. The atom's bitmask {0,1,8,11,12} is not a subset of the ESVD's bitmask {0,1,4,10,12,14}, which indicates that the ESVD is not compatible with the atom. Although

> the bonding portions are compatible, the electronic portions are not. (In general, the more fully characterized or developed an atom is, the more bits are set in its bitmask, and the less likely that the atom will be compatible with a given ESVD.)

Other evaluative action is described elsewhere in the specification, including in examples described in the specification at pp. 11 et seq. Accordingly, the rejection of claims 1-18 under 35 U.S.C. 112, first paragraph, should be withdrawn.

Claims 8 and 13-14 have been rejected under 35 U.S.C. 112, second paragraph, as being vague or indefinite with respect to "incompletely cyclic" or "extensible". For clarity, applicant has amended claims 8 and 13-14 in non-narrowing amendments for more correspondence with language indicated in the specification. As amended, claim 8 recites "acyclic" which is supported in the specification at page 32, line 3 (in connection with Fig. 20), and elsewhere. As amended, claims 13-14 recite the table being "configured to allow additional elements and values to be added", which is supported in the specification at least at page 7, lines 5-10. Applicant requests that the rejection of claims 8 and 13-14 under 35 U.S.C. 112, second paragraph, be withdrawn.

Rejections Under 35 U.S.C. 102

All of the pending claims except claims 3, 5, 9, and 12 have been rejected over Organic Chemistry, Third Edition, by Robert Thorton Morrison and Robert Neilson Boyd, copyright 1973 by Allyn and Bacon, Inc. ("the Organic Chemistry reference") at page 261 and/or page 1011.

The Organic Chemistry reference is an organic chemistry textbook that discloses chemistry principles of valence and bonding. Page 261 is directed to hydration of alkynes/tautomerism, and page 1011 is directed to structure of pyridine.

As stated in MPEP 2131:

> TO ANTICIPATE A CLAIM, THE REFERENCE MUST TEACH EVERY ELEMENT OF THE CLAIM

> "A claim is anticipated only if each and every element as set forth in the claim is found, either expressly or inherently described, in a single prior art reference." Verdegaal Bros. v. Union Oil Co. of California, 814 F.2d 628, 631, 2 USPQ2d 1051, 1053 (Fed. Cir. 1987). "The identical invention must be shown in as complete detail as is contained in the ... claim." Richardson v. Suzuki Motor Co., 868 F.2d 1226, 1236, 9 USPQ2d 1913, 1920 (Fed. Cir. 1989).

All of the claims require, among other things, both (1) analyzing a delocalized representation of a chemical structure, and (2) identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure. Pages 261 and 1011 do not teach or suggest such analysis and identification as recited in the claims. In particular, it is plain from the claims that all of the independent claims recite both delocalized and fixed bond representations of chemical structures. However, the office action makes no mention of delocalized representations, and mentions only fixed bond representations. The office action asserts only that on page 261 "a plurality of structures displaying fixed bond representation are displayed" and that on page 1011 "a plurality of structures of the pyridine ring are equivalently displayed". The office action makes no assertion at all regarding the "analyzing a delocalized representation of a chemical structure" limitation of all of the claims. While it is clear that pages 261 and 1011 disclose various chemical structures, the office action does not explain how pages 261 and 1011, together or separately, would or could anticipate the rejected claims, particularly in regard to the "analyzing a delocalized representation of a chemical structure" limitation.

Since, as stated in the MPEP as referenced above, to anticipate a claim, the reference must teach every element of the claim, applicant respectfully submits that the rejection based on the Organic Chemistry reference be withdrawn.

The dependent claims are patentable for at least the same reasons stated above.

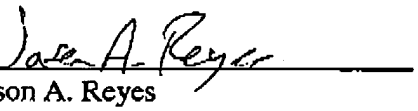
The applicant submits that the application is in condition for allowance, which action is requested.

The Examiner is encouraged to telephone the undersigned to discuss any matters in furtherance of the prosecution of the subject application.

The Commissioner is hereby authorized to charge any fee deficiency, or credit any overpayment to our Deposit Account No. 08-0219.

Respectfully submitted,

Dated: April 4, 2002



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Replacement Text for Page 5, Line 4 and Line 6 of the Specification

(MARKED TO SHOW CHANGES)

--One or more of the procedures related to dekekulization as described herein may be used in or with one or more procedures described in the following United States patent applications, which are incorporated herein: DERIVING CHEMICAL STRUCTURAL INFORMATION, serial no. [_____] 09/502,810, filed February 11, 2000, and ENHANCING STRUCTURE DIAGRAM GENERATION, serial no. [____] 09/502,133, filed February 11, 2000.--

Replacement Pages for Claims 1-18

(MARKED TO SHOW CHANGES)

1. A method for use in deriving fixed bond information, comprising:

analyzing a delocalized representation of a chemical structure;

identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

evaluating at least a subset of the fixed bond representation candidates; and

selecting from among the plurality of fixed bond representation candidates based on the evaluation.

2. A system for use in deriving fixed bond information, comprising:

an analyzer analyzing a delocalized representation of a chemical structure;

an identifier identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

an evaluator evaluating at least a subset of the fixed bond representation candidates; and

a selector electing from among the plurality of fixed bond representation candidates based on the evaluation.

3. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive fixed bond information, the instructions causing the system to:

analyze a delocalized representation of a chemical structure;

identify, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

evaluate at least a subset of the fixed bond representation candidates; and

select from among the plurality of fixed bond representation candidates based on the evaluation.

4. The method of claim 1, wherein at least a portion of the delocalized representation describes a monocyclic ring system.

5. The method of claim 1, wherein at least a portion of the delocalized representation describes a polycyclic ring system.

6. The method of claim 1, wherein at least a portion of the delocalized representation describes a ring system with a hetero substitution pattern.

7. The method of claim 1, wherein at least a portion of the delocalized representation describes a non-cyclic system.

8. The method of claim 1, wherein at least a portion of the delocalized representation describes an [incompletely cyclic] acyclic system.

9. The method of claim 1, further comprising:

including, in the produced fixed bond representation, a pair of opposite charges lacked by the delocalized representation.

10. The method of claim 1, further comprising:

including, in the produced fixed bond representation, a pair of radicals lacked by the delocalized representation.

11. The method of claim 1, further comprising:

queuing at least a subset of the candidates by priority.

12. The method of claim 1, further comprising:

using a precomputed table of atom valences as a function of element, charge, radical state, and number and distribution of bonds inside and outside of a delocalized region in the delocalized representation.

13. The method of claim 1, wherein the table [includes an extensible component] is configured to allow additional elements and values to be added.

14. The method of claim 1, wherein the table [is extensible] is configured to allow additional elements and values to be added to apply to any chemical element.

15. The method of claim 1, further comprising:

deriving electronic state and valence distributions information together with analyzing the delocalized representation.

16. The method of claim 1, further comprising:

determining whether it is practicable to produce a fixed bond representation of the chemical structure.

17. The method of claim 1, further comprising:

determining whether it is possible to produce a fixed bond representation of the chemical structure that meets a set of radicals requirements.

18. The method of claim 1, further comprising:

determining whether it is possible to produce a fixed bond representation of the chemical structure that meets a set of charges requirements.